

# Mott transitions in the multi-orbital systems

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## Abstract

We investigate the Mott transitions in the two-orbital Hubbard model with different bandwidths. By combining dynamical mean field theory with the exact diagonalization, we discuss the stability of itinerant quasi-particle states in each band. We demonstrate that separate Mott transitions occur at different Coulomb interaction strengths in general, which merge to a single transition only under special conditions. In particular, it is clarified that the  $xy$  and pair-hopping components of the Hund coupling play a key role to control the nature of the Mott transitions.

*Key words:* Mott transition, Hubbard model, Hund coupling

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Strongly correlated electron systems with multi-orbital bands pose a variety of problems. One of the interesting problems is the orbital-selective Mott transition (OSMT) in the system with distinct orbitals. The compounds  $\text{Sr}_2\text{RuO}_4$  [1,2] and  $\text{La}_{n+1}\text{Ni}_n\text{O}_{3n+1}$  [3] have the distinct type of orbitals in the  $t_{2g}$  and  $e_g$  bands, where the chemical substitution or the temperature should trigger an OSMT. [4,5] In contrast to these experimental findings, there still remains a theoretical controversy for the nature of Mott transitions in the multi-orbital system. Several groups claimed that the OSMT occurs in such a system. [6,7,8,9] On the other hand, Liebsch suggested that a single Mott transition occurs in general. [10]

A key to resolve the discrepancy may be the role played by the Hund coupling  $J$  since the nature of the Mott transition crucially depends on whether  $J$  exists or not. [8,11] As another remarkable point on the Hund coupling, it is difficult to draw a definite conclusion on the ground-state phase diagram by quantum Monte Carlo (QMC) simulations [10] since the introduction of the Hund coupling (in particular its  $xy$  and pair-

hopping components) causes serious sign problems at low temperatures.

In this paper, we revisit the OSMT in the two-orbital Hubbard model with particular emphasis on the effect of the Hund coupling. We clarify that the introduction of the anisotropy in the Hund coupling alters the nature of the Mott transitions.

Let us consider the following two-orbital Hubbard Hamiltonian at half filling,

$$\begin{aligned}
 H = & \sum_{\substack{\langle i,j \rangle \\ \alpha, \sigma}} \left( t_{ij}^{(\alpha)} - \mu \delta_{ij} \right) c_{i\alpha\sigma}^\dagger c_{j\alpha\sigma} + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} \\
 & + (U' - J) \sum_{i\sigma} n_{i1\sigma} n_{i2\sigma} + U' \sum_{i\sigma} n_{i1\sigma} n_{i2\bar{\sigma}} \\
 & - J_{xy} \sum_i \left[ c_{i1\uparrow}^\dagger c_{i1\downarrow} c_{i2\downarrow}^\dagger c_{i2\uparrow} + c_{i1\downarrow}^\dagger c_{i1\uparrow} c_{i2\uparrow}^\dagger c_{i2\downarrow} \right] \\
 & - J' \sum_i \left[ c_{i1\uparrow}^\dagger c_{i1\downarrow} c_{i2\uparrow} c_{i2\downarrow} + c_{i2\uparrow}^\dagger c_{i2\downarrow} c_{i1\uparrow} c_{i1\downarrow} \right] \quad (1)
 \end{aligned}$$

where  $c_{i\alpha\sigma}^\dagger$  ( $c_{i\alpha\sigma}$ ) creates (annihilates) an electron with spin  $\sigma$  ( $=\uparrow, \downarrow$ ) and orbital index  $\alpha$  ( $= 1, 2$ ) at the  $i$ th site and  $n_{i\alpha\sigma} = c_{i\alpha\sigma}^\dagger c_{i\alpha\sigma}$ .  $t_{ij}^{(\alpha)}$  denotes the hopping integral for orbital  $\alpha$ ,  $\mu$  the chemical potential and  $U$  ( $U'$ ) the intraband (interband) Coulomb interaction.

For the model with isotropic Hund coupling ( $J = J_{xy} = J'$ ), it was shown that the OSMTs occur for

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$J \neq 0$  in general, which merge to a single transition only at  $J = 0$  under the condition  $U = U' + 2J$ . [8] To clarify the effect of the Hund coupling in more detail, we study the roles played by the  $z$  component  $J_z (= J)$ , the  $xy$  component  $J_{xy}$ , and the pair hopping  $J'$ . In the following, we represent the two distinct electron bands by semi-circular density of states (DOS),  $\rho_\alpha(x) = 2/\pi D_\alpha \sqrt{1 - (x/D_\alpha)^2}$ , where  $2D_\alpha$  is the bandwidth.

By combining dynamical mean field theory [12] with the exact diagonalization, [13] we discuss the zero-temperature properties. To clarify the stability of the paramagnetic metallic phase, we estimate the quasi-particle weight  $Z_\alpha$  for each band ( $\alpha = 1, 2$ ), as shown in Fig. 1. When  $U = 0$ , the system is reduced to the

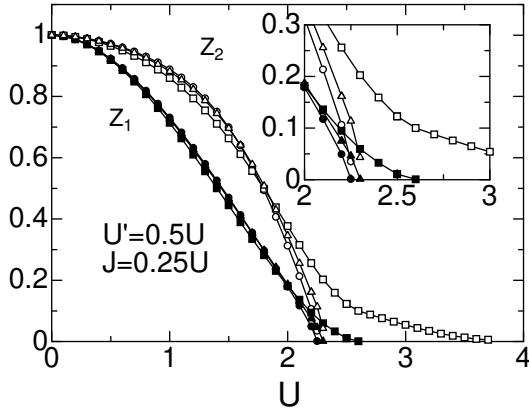


Fig. 1. Circles, triangles, and squares represent the quasi-particle weights for the case  $J_{xy}/J = J'/J = 0.0, 0.5$ , and  $1.0$  when  $U' = 0.5U$ ,  $J = 0.25U$ ,  $D_1 = 1.0$  and  $D_2 = 2.0$ .

two independent tight-binding models, where  $Z_\alpha = 1$  for each orbital. The introduction of the interactions results in the decrease of the weight for each band, for which the strong reduction appears in the narrower band ( $\alpha = 1$ ). In this parameter region, the anisotropy of the Hund coupling only weakly affects the behavior of the quasi-particle weights. However, when the system approaches the critical point, the anisotropy drastically changes the values of  $Z_\alpha$ . When the system has the isotropic interactions ( $J_{xy} = J' = J$ ), the Mott transitions occur at the different critical points depending on orbitals (i.e. OSMTs), as discussed in the previous paper. [8] On the other hand, away from the condition ( $J_{xy} = J' = J$ ), the quasi-particle weights deviate dramatically from the isotropic case, yielding very close transition points at  $J_{xy} = J' = 0$ . Therefore, we can say that the  $xy$  as well as pair-hopping components of the Hund coupling are the relevant parameters to realize the OSMT.

In this connection, we wish to mention that the present results with  $J_{xy} = J' = 0$  exhibit quite similar properties found by Liebsch with QMC for the

isotropic model with  $J = J_{xy} = J'$ , based on which he concluded that the system always undergoes the single Mott transition. [10] The present analysis would suggest that in his analysis, the effect of  $J_{xy} = J'$  gets irrelevant by some technical reason in QMC simulations, although further detailed comparison should be necessary to draw the definite conclusion.

In summary we have demonstrated that the  $xy$  and pair-hopping components of the Hund coupling are the key parameters to control the nature of the Mott transitions in the multi-orbital systems. It is an interesting problem to explore the finite temperature properties around the critical point(s) in more detail, which is now under consideration.

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